SAMMY Workshop Part 4.2c

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Part 4.2c, Formulae for Multiple Scattering Corrections

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Self-Shielding and Multiple-Scattering Corrections

See pages 201 and following in the SAMMY Users' Guide R6.
Complete documentation is in preparation.

Self-shielded capture yield:

$$Y_0 = \left(1 - \exp(-N\sigma_t Z)\right) \frac{\sigma_c}{\sigma_t}$$

N is the density (atoms/volume) of the nuclei in the sample
Z is the thickness of the sample
σ_t is the total cross section σ_c is the capture cross section

Note that there are other ways to normalize the capture yield; SAMMY has three different options. –

1. Limit as n => 0 or z => 0 = σ_c
2. $0 < Y_0 < 1$ (the version used here)
3. $0 < Y_0 < \sigma_t$ [~ (1-e) σ_c]

Single-scattering correction without edge effects
(i.e. infinite-slab approximation):

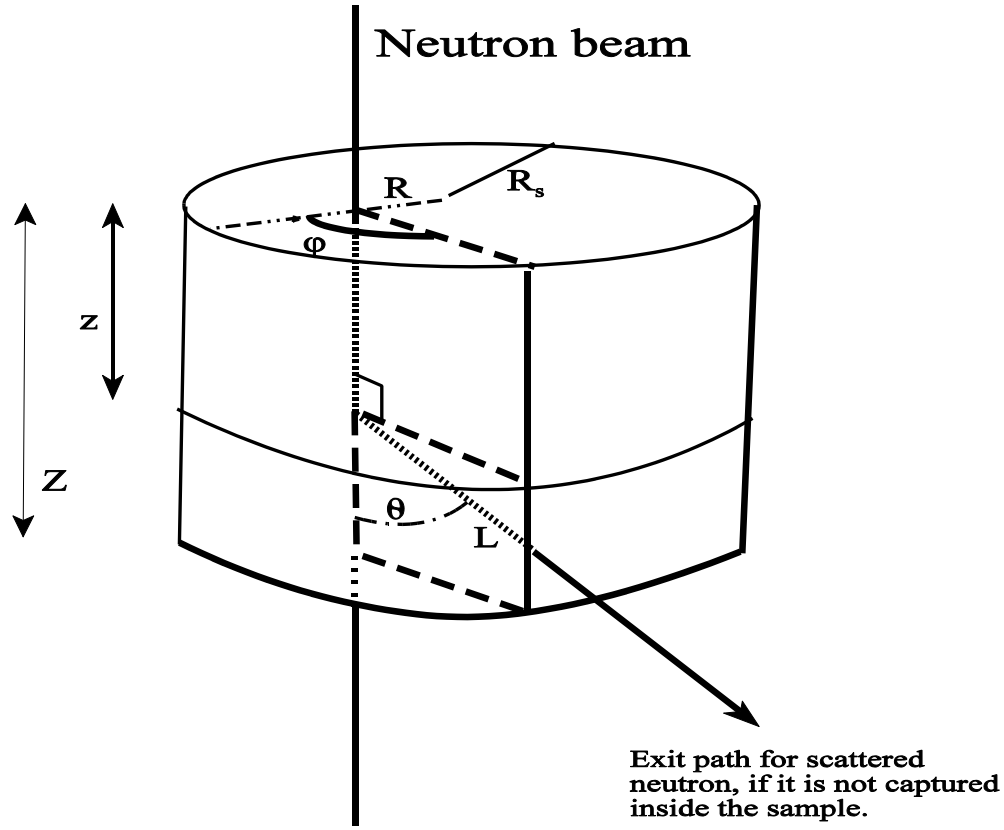
$$Y_{1\,inf} = 2\pi \int_0^1 d\mu \, \frac{\sigma_c'}{\sigma_t'} \, \frac{d\sigma}{d\Omega} \left[\frac{1 - \exp(-N\sigma_t Z)}{\sigma_t} + \frac{\exp(-N\sigma_t Z) - \exp(-N\sigma_t' Z/\mu)}{\sigma_t - \sigma_t'/\mu} \right]$$

$$+ 2\pi \int_{-1}^0 d\mu \, \frac{\sigma_c'}{\sigma_t'} \, \frac{d\sigma}{d\Omega} \left[\frac{1 - \exp(-N\sigma_t Z)}{\sigma_t} + \frac{\exp\left(-N(\sigma_t - \sigma_t'/\mu) Z\right) - 1}{\sigma_t - \sigma_t'/\mu} \right]$$

Primes indicate quantities are to be evaluated at the scattered energy:

$$E' = E \left[\frac{\cos\theta}{(1+r)} + \sqrt{\frac{1}{(1+1/r)^2} - \frac{\sin^2\theta}{(1+r)^2}} \right]^2$$

where r is ratio of mass of nucleus to mass of neutron, and $\cos\theta = \mu$.



Geometry for the single-scattering correction to capture or fission yield, for a neutron incident on the flat side of a cylindrical sample.

Edge-effects correction for Cylinder:

$$Y_{1ec} = \int_0^{\mu_1} d\mu \; \frac{d\sigma}{d\Omega} \; \frac{\sigma_c'}{\sigma_t'} \; Q_f(\mu, \sigma_t, \sigma_t') + \int_{-\mu_1}^{0} d\mu \; \frac{d\sigma}{d\Omega} \; \frac{\sigma_c'}{\sigma_t'} \; Q_b(-\mu, \sigma_t, \sigma_t')$$

where Q_f and Q_b are defined as

$$Q_f(\mu, \sigma_t, \sigma_t') = \int_0^{z_1} dz \; \exp(-N\sigma_t z) \; U(\mu, z, \sigma_t')$$

$$Q_b(\mu, \sigma_t, \sigma_t') = \int_0^{z_1} dz \; \exp\left(-N\sigma_t (Z-z)\right) U(-\mu, z, \sigma_t')$$

with U given by

$$U(\nu,w,s) = -\frac{4N}{R_0^2}\int_{R_1}^{R_0} R\,dR \int_0^{\varphi_1} d\varphi \left(\exp\left(-\frac{Ns(Z-w)}{\nu} \right) \right.$$

$$\left. - \exp\left(-\frac{Ns\left(-R\cos\varphi + \sqrt{R_s^2 - R^2\sin^2\varphi} \right)}{\sqrt{1-\nu^2}} \right) \right)$$

The limits in these expressions are given by

$$\mu_1 = \cos\theta_1 \qquad \tan\theta_1 = (R_s - R_0)/Z$$

$$z_1 = Z - (R_s - R_0)/\tan\theta \qquad R_1 = R_s - (Z-z)\tan\theta$$

$$\cos\varphi_1 = \frac{R_s^2 - R^2 - (Z-z)\tan^2\theta}{2\,(Z-z)\,R\tan\theta}$$

Multiple*Scattering Correction for Capture and Fission Yield

* "Multiple" => Double, Triple, etc.

Treatment borrowed from M. Moxon, REFIT

- <u>Assumption</u>: after a few scatterings, neutrons are distributed uniformly throughout the sample, and directions of motion are also distributed uniformly

- Probability of escape for neutron after k scatters is $e^{-N\sigma^k L}$ where L is distance left to travel

- Average escape probability is therefore

$$p_e(E^{(k)}) = \frac{1}{ZN\sigma^{(k)}} \left[\frac{1}{2} - \int_1^{inf} u^{-3}\, du\; e^{-N\sigma^{(k)} Zu} \right]$$

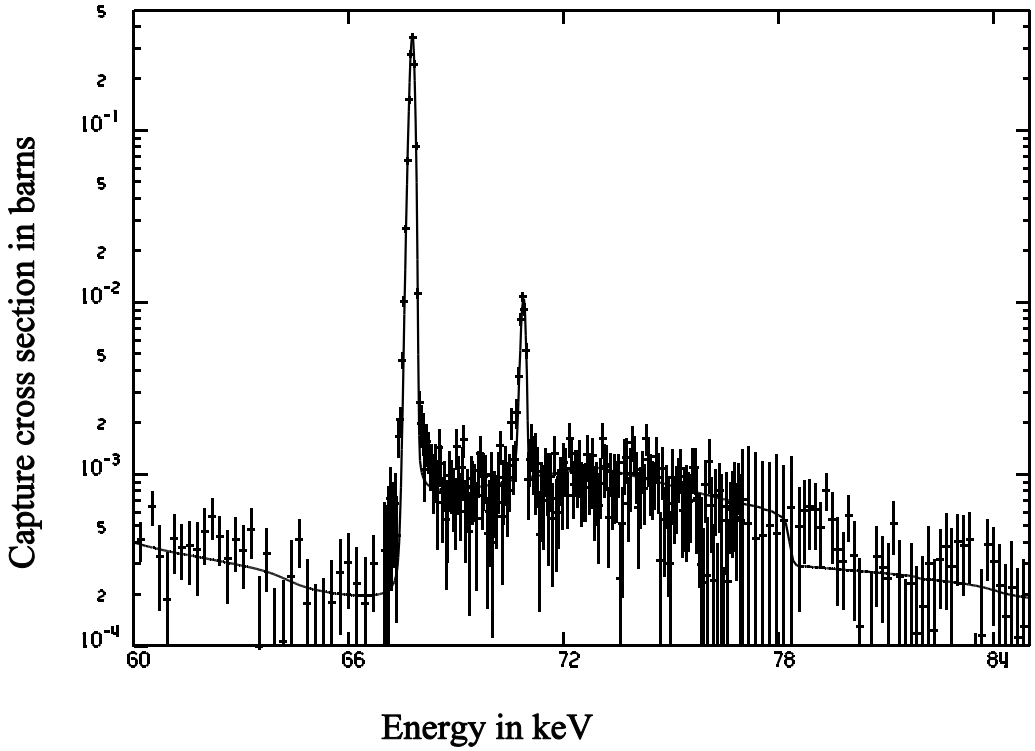
- Correction for capture preceded by 2, 3, 4, ... scatterings is given by

$$\bar{Y}_2(E) = N \int dz\; e^{-N\sigma_t z}\; 2\pi N \int d\mu_1\; \frac{d\sigma}{d\Omega_1}\; y_1 \int dq_1\; e^{-N\sigma_t' q_1}$$

where y_i are found iteratively from

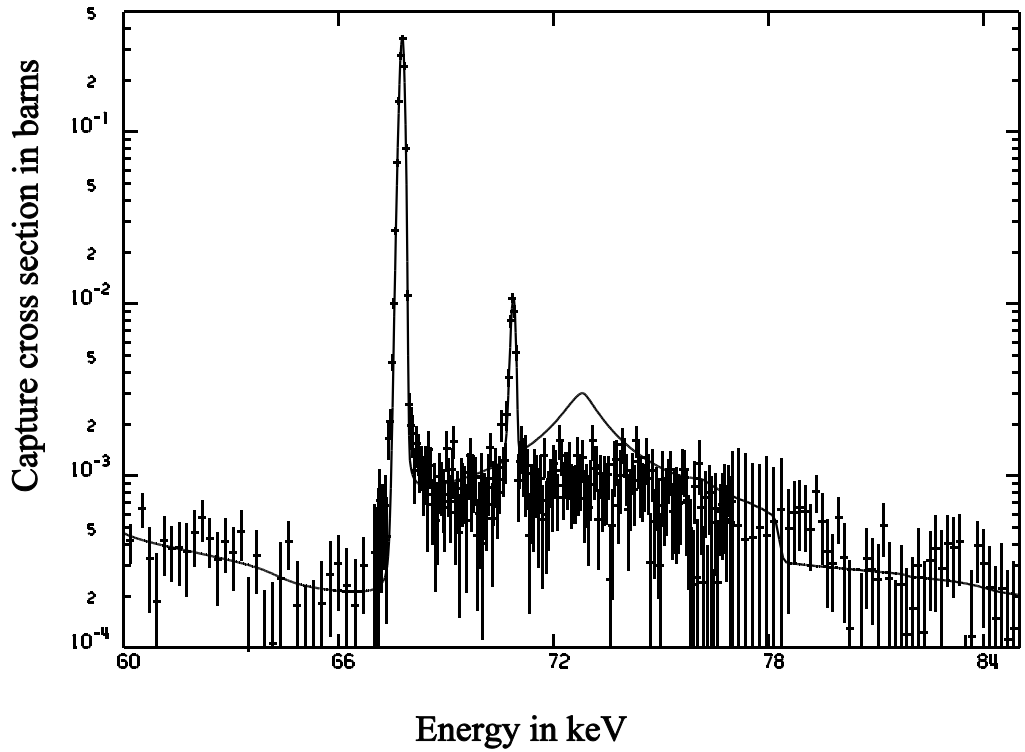
$$y_{j-1} = 2\pi \int d\mu_j\; \frac{d\sigma^{(j-1)}}{d\Omega_j} \left(\sigma_c^{(j)} + y_j \right) \left(1 - p_e(E^{(j)}) \right)$$

(Superscript j on cross sections indicates that cross section is to be evaluated at the energy after j scatters.)



Doing It Right

Crosses are measured natural Si data of Guber (ORNL). Solid curve is SAMMY calculation using full finite-size corrections (self-shielding, single-scattering with edge effects, and double-plus scattering).



Using an approximation that often works fine

Crosses are measured natural Si data of Guber (ORNL); solid curve is SAMMY calculation using some finite-size corrections (self-shielding, single-scattering in infinite-slab approximation, and double-plus scattering).

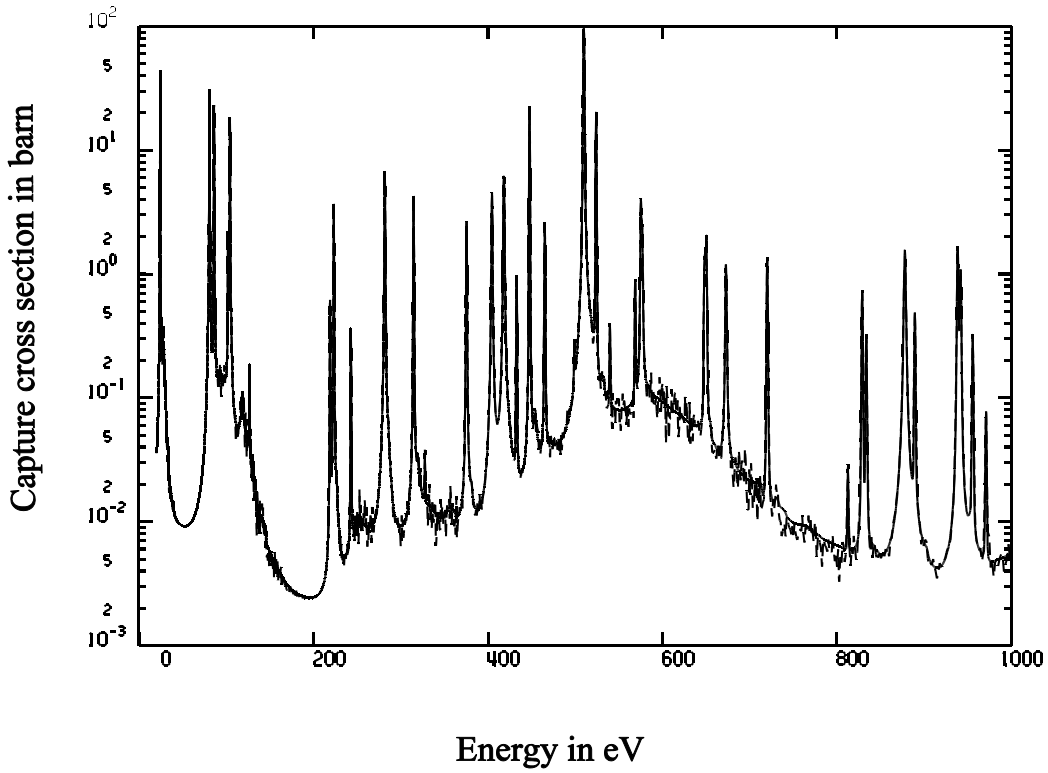
Question: Are the SAMMY multiple-scattering corrections correct?

Answer: Maybe!

- When approximations are good, computed corrections should be good.
- Otherwise, maybe not.

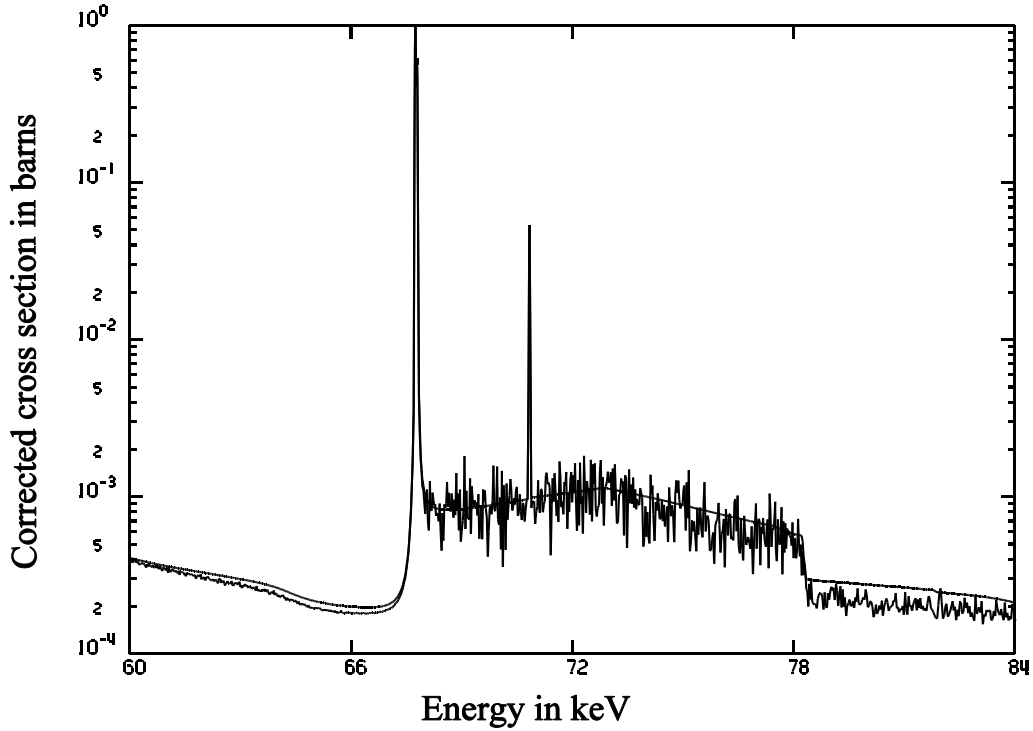
For a particular case,
how do we know for sure?

- Do Monte-Carlo simulations (use code SAMSMC)
- Start from same Doppler-broadened cross sections for both SAMMY and Monte-Carlo



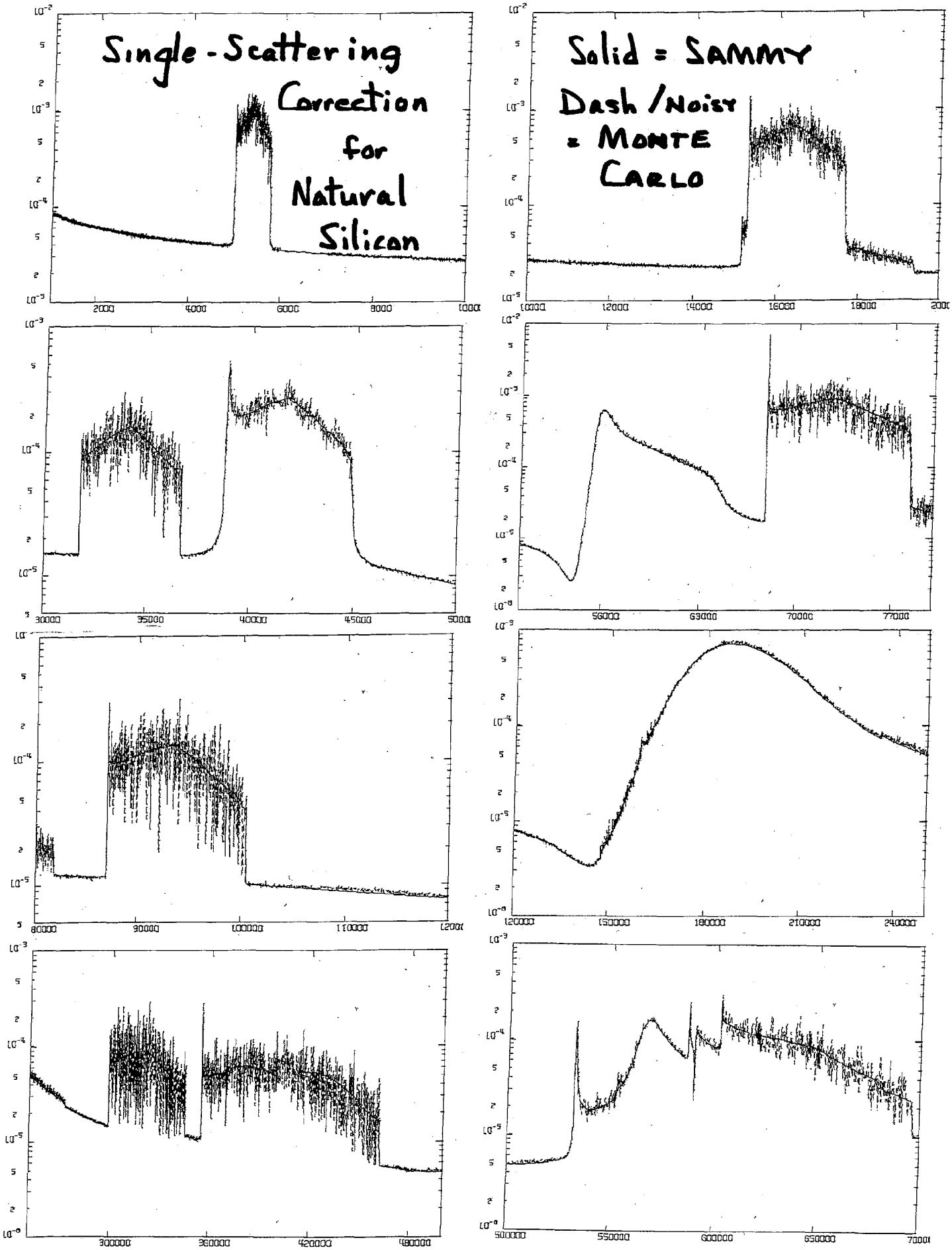
Calculation of corrected capture cross section for $BaCO_3$. Corrections include self-shielding and multiple scattering, assuming the sample is a finite cylindrical disk. The dashed curve is the preliminary Monte-Carlo calculation (averaged by 5), and the solid curve is the SAMMY formulation.

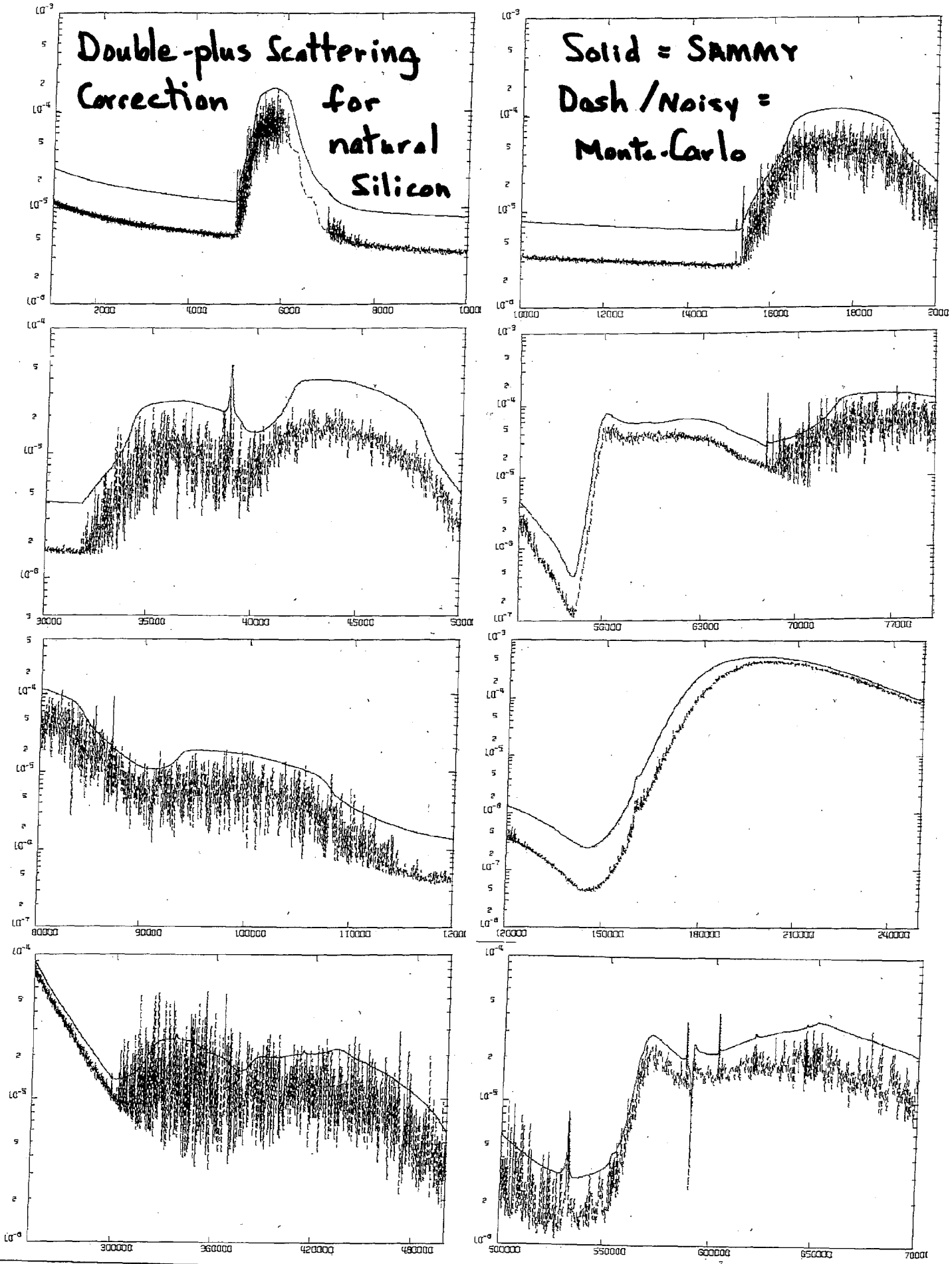
(Data of Paul Koehler et al. are not shown, as this calculation does not include resolution broadening, normalization, or background.)

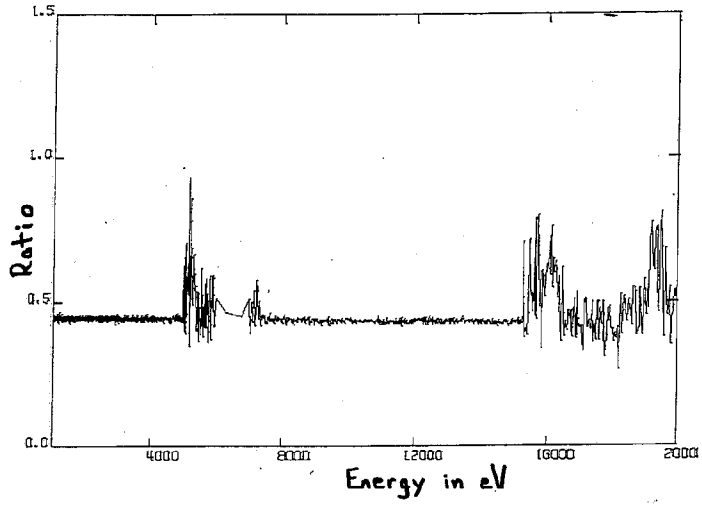


SAMMY calculation (smooth curve)
vs preliminary Monte-Carlo calculation (structured curve)
for capture cross section of natural Si.

The included corrections are self-shielding, single-scattering with edge effects, and double-plus scattering. Cross sections were Doppler-broadened before multiple-scattering corrections were applied; no resolution broadening was used.

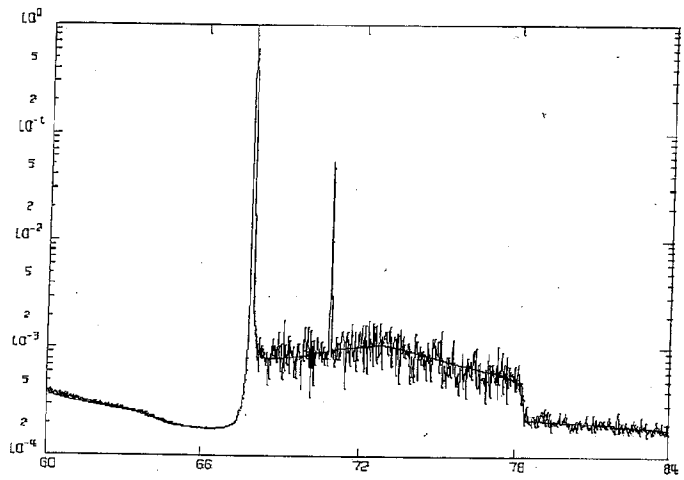

Single-Scattering Correction for Natural Silicon
Solid = SAMMY
Dash / Noisy = MONTE CARLO


Double-plus Scattering Correction for natural Silicon
Solid = SAMMY
Dash / Noisy = Monte-Carlo

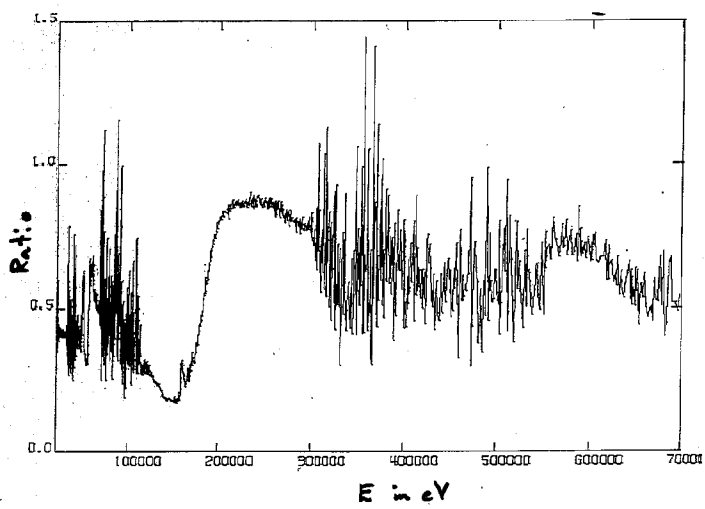


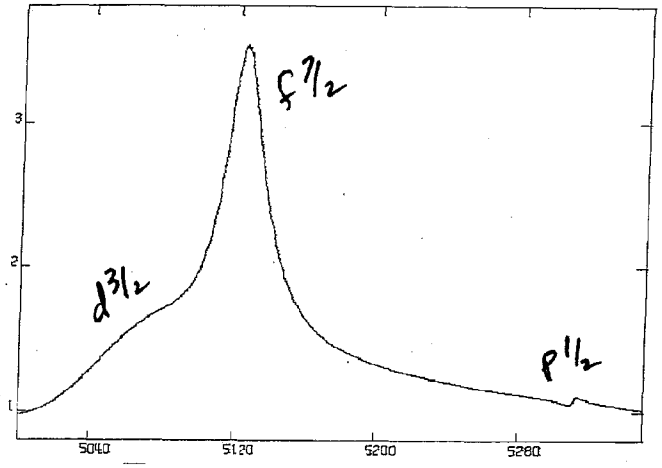
$$\text{Ratio} = \frac{\text{Monte-Carlo double-plus}}{\text{SAMMY double-plus}}$$

for natural Silicon



with 0.44 fudge factor on Y2

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p 1/2
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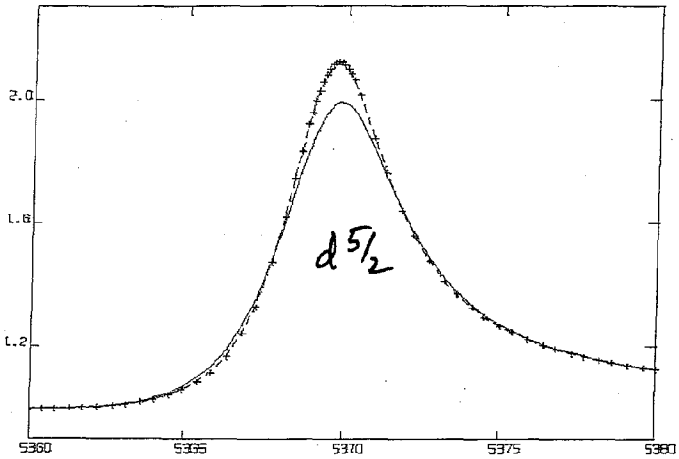
5120
5200
5280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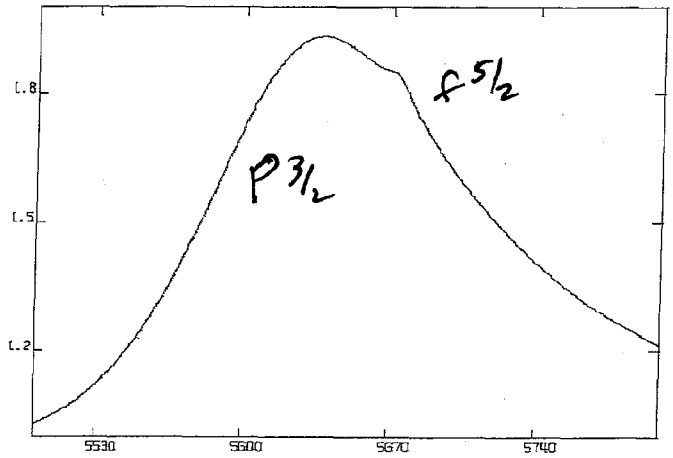
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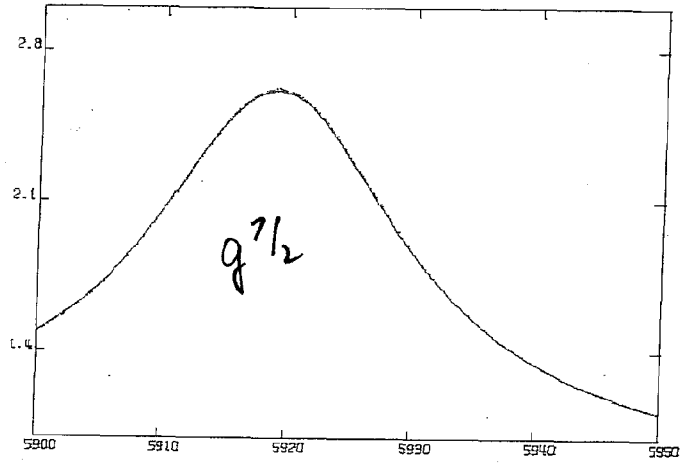
5670
5740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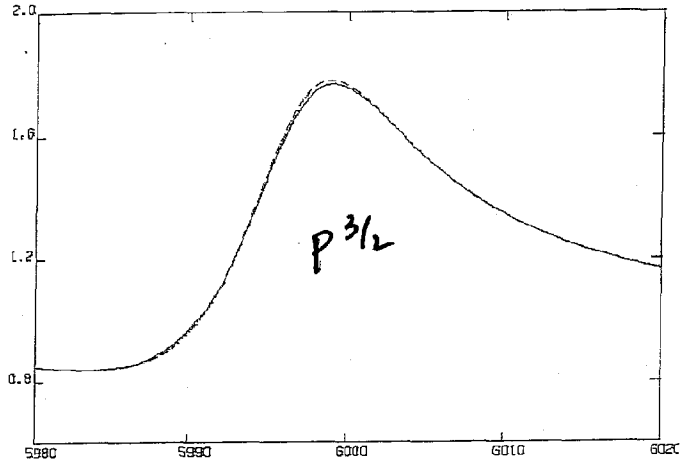
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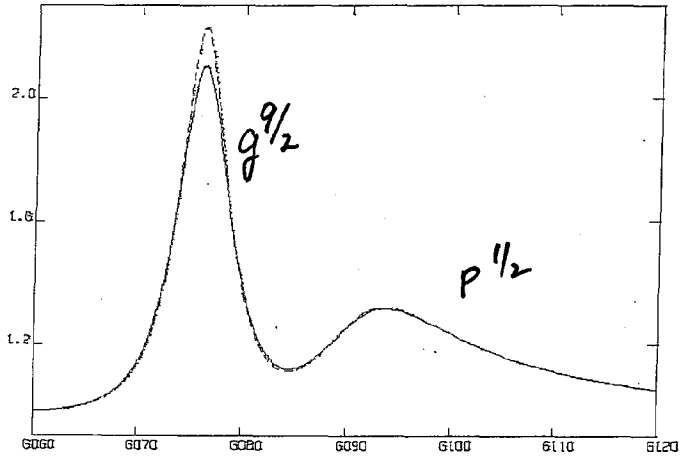
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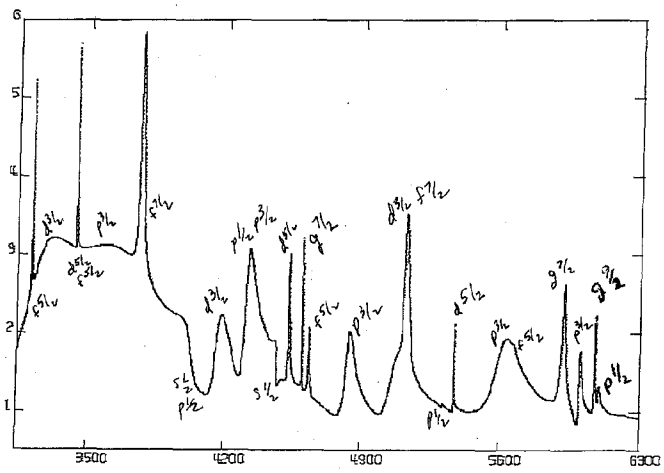
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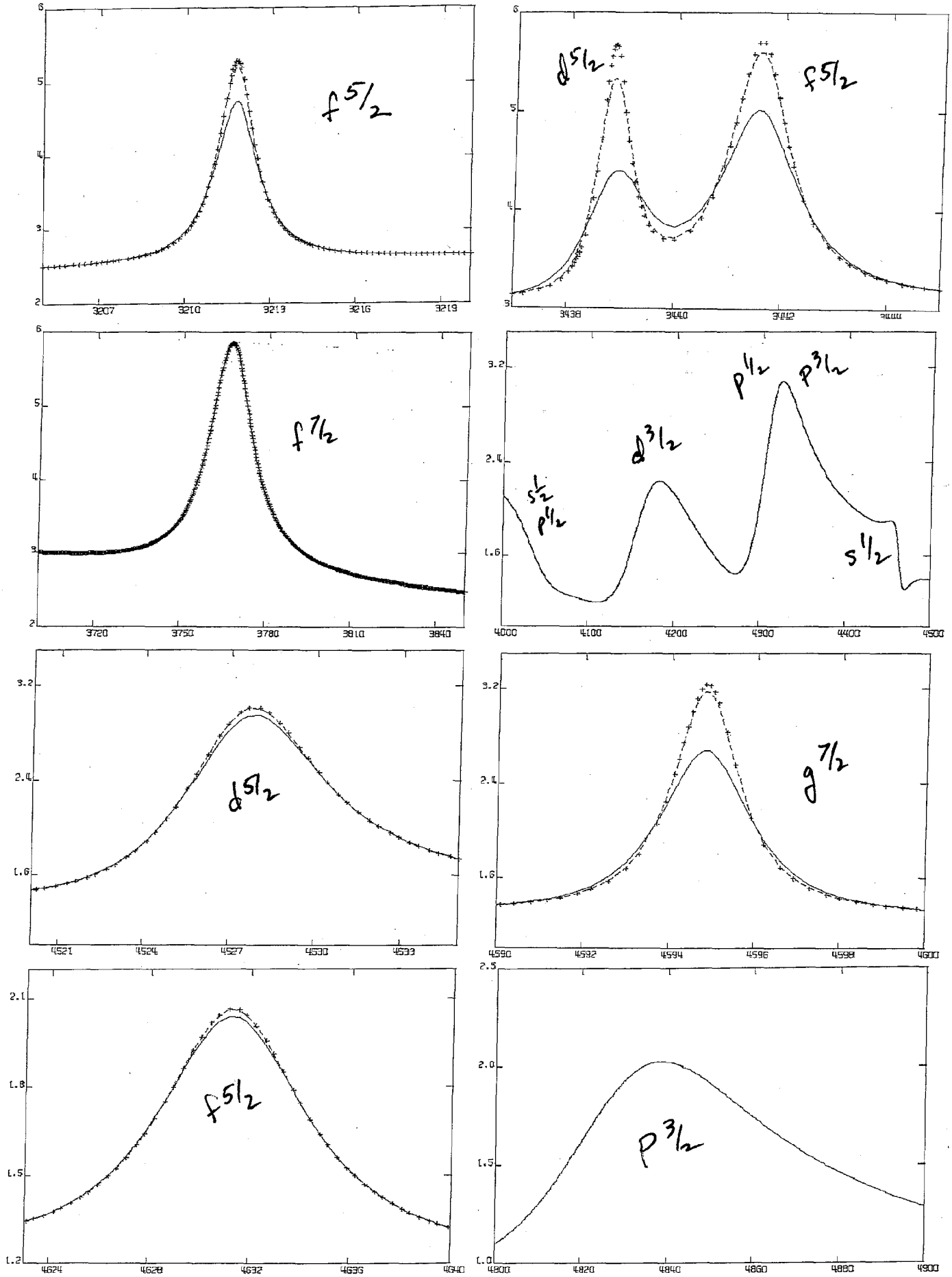
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d 5/2
f 5/2
f 7/2
s 1/2
p 1/2
d 3/2
p 1/2
p 3/2
s 1/2
d 5/2
g 7/2
f 5/2
p 3/2

NOTE: For multiple-scattering (and in general), SAMMY will calculate what you tell it to calculate.

"Garbage in / Garbage out" applies here!

EXAMPLE: 1.15-keV p-wave resonance in Fe56

"SAMMY is not giving the single-scattering peak, we can't figure out why."

Top part of PAR file:

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(blank)
(blank)
NORMALIZATION AND BACKGROUND
   700000.     4500.              ...       1 1
    10000.     1000.
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Bottom part of INPut file:

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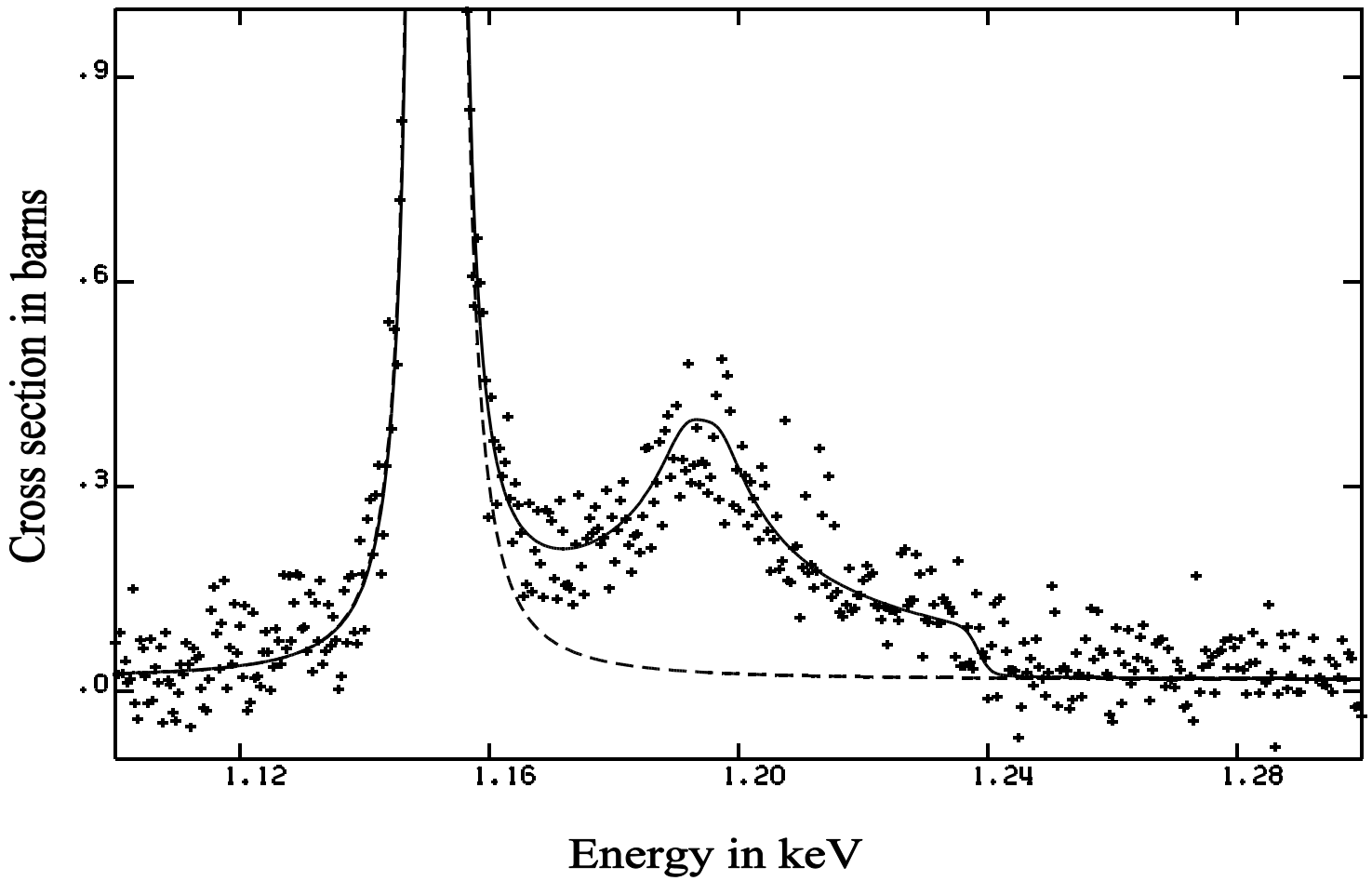
CAPTURE
        0.0        0.0     0     1
  1       1     0 -0.5        1.0
    1     1     0     1        0.5
(blank)
      0.15        1.0                  0.0
```

Can you tell what's missing?



The 1.15-keV ^{56}Fe resonance in natural iron capture data of R. Spencer et al. Dashed curve is SAMMY calculation using the input on the previous page; solid curve is correct calculation of single-scattering correction.